

Manipulating the electron current through a splitting

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Abstract

The description of electron current through a splitting is a mathematical problem of electron transport in quantum networks [5, 1]. For quantum networks constructed on the interface of narrow-gap semiconductors [30, 2] the relevant scattering problem for the multi-dimensional Schrödinger equation may be substituted by the corresponding problem on a one-dimensional linear graph with proper self-adjoint boundary conditions at the nodes [10, 9, 26, 25, 17, 20, 4, 29, 21, 19, 6, 5, 1]. However, realistic boundary conditions for splittings have not yet been derived.

Here we consider some compact domain attached to a few semi-infinite lines as a model for a quantum network. An asymptotic formula for the scattering matrix for this object is derived in terms of the properties of the compact domain. This allows us to propose designs for devices for manipulating quantum current through a splitting [3, 15, 23, 11, 22].

Introduction: current manipulation in the resonance case

In this paper we discuss the scattering problem on a compact domain with a few semi-infinite wires attached. This is motivated by the design of quantum electronic devices for triadic logic. In the papers [3, 15] a special design of the one-dimensional graph which permits manipulation of the current through an elementary ring-like splitting is suggested. This permits, *in principle*, manipulation of quantum current in the resonance case to form a quantum switch. Another device for manipulating quantum current through splittings is discussed in [23, 11]. In [22] the special design of the splitting formed as a circular domain with four one-dimensional wires attached is used to produce a triadic relay.

In order to illustrate the basic principle of operation consider the self-adjoint Schrödinger operator

$$\begin{cases} \mathcal{L} \equiv -\Delta + q(x) \\ \frac{\partial \Psi}{\partial n}|_{\partial\Omega} = 0. \end{cases}$$

on some compact domain Ω . In this paper we will only consider the case $\Omega \subset \mathbb{R}^3$ [23] (for other cases see also [3, 15, 22]). Roughly speaking the solution of the Cauchy problem

$$\begin{cases} \frac{\partial \Psi}{i\partial t} = \mathcal{L}\Psi \\ \Psi(x, 0) = \Psi_0(x) \end{cases} \quad (1)$$

is given in terms of eigenfunctions φ_n

$$\Psi(x, t) = \sum_n \alpha_n e^{i\lambda_n t} \varphi_n(x).$$

Picking a specific mode φ_0 with energy λ_0 we suppose that φ_0 disappears on some subset $l_0 \subset \Omega$. Connecting ‘thin channels’ at various points on the

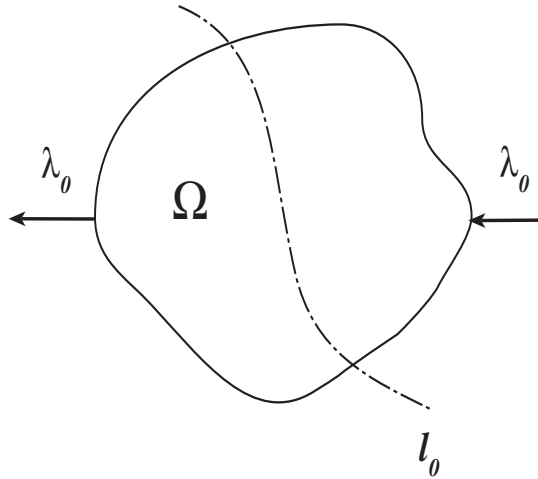


figure 1. Resonance switch

boundary of Ω and introducing an excitation of energy λ_0 along the channels we can hope to create a switching effect. Essentially this is achieved by varying $q(x)$ so that $l_0 \cap \partial\Omega$ coincides with the connection point of a ‘thin channel’.

Implicit in our construction is the assumption that the energy of the electrons in the device is equal to some resonance eigenvalue of the Schrödinger operator on Ω . We refer to this as the *resonance case*¹.

Another assumption which we have made above is that λ_0 is a *simple* eigenvalue of \mathcal{L} . We will show that the case of multiple eigenvalues is a simple generalisation of the case for simple eigenvalues, see [3, 15].

In the first section we give a brief description of the connection of the thin channels (here they are modelled by one-dimensional semi-lines) to the compact domain, for more details see [23]. In the second section we derive an asymptotic formula for the scattering matrix in terms of the eigenfunctions on the compact domain. In the last section we briefly discuss some simple models of a quantum switch constructed on the basis of this asymptotic formula.

¹This has interesting implications when we consider the effect of decreasing the length scale—or equivalently scaling up the energy—viz. the effect of non-zero temperature becomes negligible for sufficiently small length scales, see [14].

1 Connection of compact domain to thin channels

As we mentioned above the thin channels are modelled by one-dimensional semi-lines. This is justified by an appropriate choice of materials (narrow-band semiconductors) and energies, see [30, 2, 22]. We assume that these channels are attached at the points $\{a_1, a_2, \dots, a_N\} \subset \partial\Omega$ (perturbation of the operator \mathcal{L} at inner points $\{a_{N+1}, a_{N+2}, \dots, a_{N+M}\}$ may be considered using the same techniques as for $\{a_1, a_2, \dots, a_N\}$ [2, 3, 22] although we do not consider this here).

We refer to \mathcal{L} , defined above, as the *unperturbed* Schrödinger operator. \mathcal{L} is restricted to the symmetric operator \mathcal{L}_0 defined on the class D_0 of smooth functions with Neumann boundary conditions which vanish near the points a_1, a_2, \dots, a_N . The deficiency subspaces, $\mathcal{N}_{\pm i}$, of the restricted symmetric operator \mathcal{L}_0 ,

$$[\mathcal{L}_0^* \pm i] e_{\pm i}^s = 0$$

for complex values of the spectral parameter λ coincide with Greens functions $G_\lambda(x, a_s)$ of \mathcal{L} which are elements of $L_2(\Omega)$ but do not belong to the Sobolev class $W_2^1(\Omega)$. In the case when Ω is a compact one-dimensional manifold (a compact graph) these Greens functions are continuous and can be written in terms of a convergent spectral series [3]. However, when $\Omega \subset \mathbb{R}^2, \mathbb{R}^3$ the deficiency elements will have singularities and we must use an iterated Hilbert identity to regularise the values of the Greens function at the poles.

It is well known, for $\Omega \subset \mathbb{R}^3$, that the Greens function admits the representation inside Ω

$$G_\lambda^0(x, y) = \frac{e^{i\sqrt{\lambda}|x-y|}}{4\pi|x-y|} + g(x, y, \lambda) \quad (2)$$

where $g(x, y, \lambda)$ is continuous. The potential-theory approach gives the asymptotics of the Green function near the boundary point $a_s \in \partial\Omega$

$$G_\lambda^0(x, a_s) \sim \frac{1}{2\pi|x-a_s|} + L_s(x) + B_s(x, \lambda), \quad (3)$$

where L_s is a logarithmic term depending only on $\partial\Omega$ and B_s is a bounded term containing spectral information [8].

In order to choose regularised boundary values we use the following lemma [23] (here we assume $\mathcal{L} > -1$ is semi-bounded from below):

Lemma 1 *For any regular point λ from the complement of the spectrum $\sigma(\mathcal{L})$ of \mathcal{L} and any $a \in \{a_s\}_{s=1}^{N+M}$ the following representation is true:*

$$G_\lambda(x, a) = G_{-1}(x, a) + (\lambda + 1)G_{-1} * G_\lambda(x, a),$$

where the second addend is a continuous function of x and the spectral series of it in terms of eigenfunctions φ_l of the nonperturbed operator \mathcal{L}

$$(\lambda + 1)G_{-1} * G_\lambda(x, a) = (\lambda + 1) \sum_l \frac{\varphi_l(x)\varphi_l(a)}{(\lambda_l + 1)(\lambda_l - \lambda)}$$

is absolutely and uniformly convergent in Ω .

The proof of this lemma is based on the classical Mercer theorem along with the Hilbert identity [23].

It is well known that the domain of \mathcal{L}_0^* can be written as the direct sum

$$D_0^* = D_0 + \mathcal{N}_i + \mathcal{N}_{-i} \quad (4)$$

so for any $u \in D_0^*$

$$u = u_0 + \sum_s A_s^+ G_i(x, a_s) + \sum_s A_s^- G_{-i}(x, a_s).$$

We define $u \in D_0^*$ in terms of the coordinates

$$\begin{aligned} A_s &\equiv A_s^+ + A_s^-, \\ B_s &\equiv \lim_{x \rightarrow a_s} \left[u(x) - \sum_t A_t \Re G_i(x, a_t) \right], \end{aligned}$$

the *singular* and *regular* amplitudes respectively since it is clear from the above lemma that A_s is the coefficient of the singular part and B_s the coefficient of the regular part of $u \in D_0^*$. The boundary form of \mathcal{L}_0^* may be written in terms of A_s B_s as a hermitian symplectic form

$$\langle \mathcal{L}_0^* u, v \rangle - \langle u, \mathcal{L}_0^* v \rangle = \sum B_s^u \bar{A}_s^v - A_s^u \bar{B}_s^v. \quad (5)$$

1.1 Self-adjoint extensions

We recall that to each boundary point a_s , $s = 1, \dots, N$, there is attached a semi-infinite ray. On the s -th ray we define the symmetric operator

$$l_{s,0} = -\frac{d^2}{dx_s^2} + q_s(x_s),$$

on functions which vanish at $x_s = 0$ (which is identified with $a_s \in \Omega$).

Let us consider the symmetric operator $\mathcal{L}_0 \oplus l_{1,0} \oplus l_{2,0} \oplus \dots \oplus l_{N,0}$. The connection between the compact domain and the rays is given by (a particular) self-adjoint extension of this operator. The boundary form of the adjoint $\mathcal{L}_0^* \oplus l_{1,0}^* \oplus l_{2,0}^* \oplus \dots \oplus l_{N,0}^*$ is easily seen to be

$$\sum_s^N (B_s^u \bar{A}_s^v - A_s^u \bar{B}_s^v) + \sum_s^N (u_s'(0) \bar{v}_s(0) - u_s(0) \bar{v}_s'(0)). \quad (6)$$

It is well known that the self-adjoint extensions of $\mathcal{L}_0 \oplus l_{1,0} \oplus l_{2,0} \oplus \dots \oplus l_{N,0}$ correspond to Lagrange planes in the Hermitian symplectic space of boundary values equipped with the above boundary form [27]. In general, if A, B are (vectors of) boundary values for some symmetric operator then any self-adjoint extension can be described by

$$\frac{i}{2}(U - \mathbb{I})A + \frac{1}{2}(U + \mathbb{I})B = 0$$

for some unitary matrix U [14, 13].

We choose the particular family of self-adjoint extensions which correspond to the following boundary conditions at the N points of contact of the rays

$$\begin{pmatrix} A_s \\ u_s(0) \end{pmatrix} = \begin{pmatrix} 0 & \beta \\ \beta & 0 \end{pmatrix} \begin{pmatrix} B_s \\ u'_s(0) \end{pmatrix}, \quad (7)$$

for $s = 1, \dots, N$ and $\beta > 0$. The resulting self-adjoint extension we denote by \mathcal{L}_β . The parameter β is a measure of the strength of the connection between the rays and the compact domain—in the limit $\beta \rightarrow 0$ the resolvent of \mathcal{L}_β converges uniformly to the resolvent of \mathcal{L} on each compact subset of the resolvent set of \mathcal{L} [23].

2 Asymptotics of the scattering matrix

For the remainder we assume that the potential on the rays $q_s(x_s) \equiv 0$ is zero.

We use the ansatz

$$u_s = f_s(x_s, -k)\delta_{s1} + f_s(x_s, k)S_{s1}, \quad (8)$$

for the scattered wave generated by the incoming wave from the ray attached to the point a_1 . Here $f_s(x_s, \pm k)$ are the Jost solutions [28], in this case ($q_s(x_s) \equiv 0$) just the exponentials

$$f_s(x_s, \pm k) = e^{\pm ikx_s},$$

and $\lambda = k^2$ is the spectral parameter.

From the boundary conditions (7) we get N equations

$$\begin{aligned} A_s &= \beta f'_s(0, -ik)\delta_{s1} + \beta f'_s(0, ik)S_{s1} \\ \beta B_s &= f_s(0, -ik)\delta_{s1} + f_s(0, ik)S_{s1}. \end{aligned} \quad (9)$$

Inside Ω the eigenfunction $u(x, k)$ may be written as a sum of Greens functions at the spectral parameter $\lambda = k^2$

$$u(x, k) = \sum_s^N C_s G_\lambda(x, a_s).$$

Using the Cayley transform between the spectral points i and λ one gets a relationship between these Greens functions and the deficiency elements (as defined above) so that [23]

$$\lim_{x \rightarrow a_s} [G(x, a_s, \lambda) - \Re G(x, a_s, i)] = \left(\frac{\mathbb{I} + \lambda \mathcal{L}}{\mathcal{L} - \lambda \mathbb{I}} G_i(a_s), G_i(a_s) \right) \equiv g^s(\lambda).$$

Consequently we can show that u has the following asymptotics as $x \rightarrow a_s$

$$u \sim C_s \Re G_i(x, a_s) + C_s g^s(\lambda) + \sum_{t \neq s} C_t G_\lambda(a_s, a_t) + o(1). \quad (10)$$

It follows that for the scattering wave the symplectic variables are related by

$$\begin{aligned} A_s &= C_s \\ B_s &= g^s(\lambda)C_s + \sum_{t \neq s} C_t G_\lambda(a_s, a_t), \end{aligned}$$

that is $B = QA$ where

$$Q(\lambda) = \begin{pmatrix} g^1(\lambda) & G_\lambda(a_1, a_2) & \cdots & G_\lambda(a_1, a_N) \\ G_\lambda(a_2, a_1) & g^2(\lambda) & \cdots & G_\lambda(a_2, a_N) \\ \vdots & & \ddots & \vdots \\ G_\lambda(a_N, a_1) & \cdots & \cdots & g^N(\lambda) \end{pmatrix}. \quad (11)$$

Putting this into (9) we can solve for the scattering matrix to get

$$S = -\frac{\mathbb{I} + ik\beta^2 Q}{\mathbb{I} - ik\beta^2 Q}. \quad (12)$$

Let us choose an eigenvalue λ_0 of the unperturbed operator \mathcal{L} on Ω . We suppose that λ_0 has a p -dimensional eigenspace, which we denote \mathcal{R}_0 , with orthonormal basis $\{\varphi_{0,i}\}^p$. The following important technical statement close to Lemma 1 above is true [23]:

Theorem 1 *The elements of the Q -matrix have the following asymptotics at the spectral point λ_0 :*

$$Q_{st}(\lambda) \sim \sum_{i=1}^p \frac{\varphi_{0,i}(a_s)\varphi_{0,i}(a_t)}{\lambda_0 - \lambda} + \mathcal{Q}_0(a_s, a_t, \lambda),$$

where $\mathcal{Q}_0(a_s, a_t, \lambda)$ is a continuous function at the point $\lambda = \lambda_0$.

We will use this result to prove an asymptotic formula for the scattering matrix in the limit of weak connection between the compact domain and the rays.

Consider the mapping $\mathcal{P} : L_2(\Omega) \rightarrow \mathbb{C}^N$ which gives the vector of values of a function in $L_2(\Omega)$ at the nodes of each of the N rays. To distinguish between functions and elements of \mathbb{C}^N we use the notation

$$\mathcal{P}(\psi) = |\psi\rangle \in \mathbb{C}^N,$$

and we denote

$$R_0 \equiv \mathcal{P}(\mathcal{R}_0).$$

Proposition 1 *It is possible to choose an orthonormal basis $\{\phi_{0,i}\}^p$ for \mathcal{R}_0 which forms an orthogonal, but not necessarily normalised, basis for R_0 under \mathcal{P} .*

Proof: Given some orthonormal basis $\{\varphi_{0,i}\}^p$ for \mathcal{R}_0 we see that

$$\phi_{0,i} = \sum_{j=1}^p U_{ij} \varphi_{0,j}$$

is also an orthonormal basis where $U \in \mathbf{U}(p)$.
The inner product of the image under P

$$\langle \phi_{0,i} | \phi_{0,j} \rangle = \sum_{r,s=1}^p \bar{U}_{ir} \langle \varphi_{0,r} | \varphi_{0,s} \rangle U_{js}$$

shows that finding an *orthogonal* basis for \mathcal{R}_0 amounts to finding the unitary matrix U which diagonalises $A_{rs} = \langle \varphi_{0,r} | \varphi_{0,s} \rangle$. \square

This allows us to write Q in ‘diagonal’ form

$$\begin{aligned} Q &= \frac{1}{\lambda_0 - \lambda} [|\phi_{0,1}\rangle \langle \phi_{0,1}| + \cdots + |\phi_{0,m}\rangle \langle \phi_{0,m}|] \\ &\quad + \mathcal{Q}_0(\lambda) \\ &= \frac{D_l}{\lambda_0 - \lambda} + \mathcal{Q}_0(\lambda) \end{aligned} \tag{13}$$

where $m \leq p$ is the dimension of R_0 .

Theorem 2 *If λ_0 is an eigenvalue of \mathcal{L} then for vanishing coupling $\beta \sim 0$ the scattering matrix of \mathcal{L}_β has the form*

$$\begin{aligned} S(\lambda_0) &= -\mathbb{I} + 2P_0 - 2 \sum_{s=1} (ik_0 \beta^2 P_0^\perp \mathcal{Q}_0 P_0^\perp)^s \\ &= -\mathbb{I} + 2P_0 + O(\beta^2) \end{aligned} \tag{14}$$

where P_0 is the orthogonal projection onto R_0 .

Proof: Using equation (13),

$$S(\lambda) = - \left[\mathbb{I} + \frac{ik\beta^2 D_0}{\lambda_0 - \lambda} + ik\beta^2 \mathcal{Q}_0 \right] \left[\mathbb{I} - \frac{ik\beta^2 D_0}{\lambda_0 - \lambda} - ik\beta^2 \mathcal{Q}_0 \right]^{-1}.$$

Since $D_0 = D_0^\star$, the matrix $E_0 = \mathbb{I} - \frac{ik\beta^2 D_0}{\lambda_0 - \lambda}$ is invertable. Consequently the denominator can be written

$$\begin{aligned} \left[\mathbb{I} - \frac{ik\beta^2 D_0}{\lambda_0 - \lambda} - ik\beta^2 \mathcal{Q}_0 \right]^{-1} &= [\mathbb{I} - ik\beta^2 \mathcal{Q}_0 E_0^{-1}] E_0^{-1} \\ &= E_0^{-1} [\mathbb{I} - ik\beta^2 \mathcal{Q}_0 E_0^{-1}]^{-1}. \end{aligned}$$

Again the matrix $\mathbb{I} - ik\beta^2 \mathcal{Q}_0 E_0^{-1}$ has an inverse for $\lambda \sim \lambda_0$ since $\mathcal{Q}_0 = \mathcal{Q}_0^\star$. This gives the following expression for the scattering matrix

$$\begin{aligned} S(\lambda) &= - [E_0^\star E_0^{-1} + ik\beta^2 \mathcal{Q}_0 E_0^{-1}] [\mathbb{I} - ik\beta^2 \mathcal{Q}_0 E_0^{-1}]^{-1} \\ &= - [E_0^\star E_0^{-1} + ik\beta^2 \mathcal{Q}_0 E_0^{-1}] \sum_{s=0} (ik\beta^2 \mathcal{Q}_0 E_0^{-1})^s. \end{aligned}$$

Denoting $\pi_i \equiv \sqrt{\langle \phi_{0,i} | \phi_{0,i} \rangle}$ and diagonalising we can write,

$$\begin{aligned} E_0^{-1} &= \text{diag} \left(1 - \frac{ik\beta^2\pi_1^2}{\lambda_0 - \lambda}, \dots, 1 - \frac{ik\beta^2\pi_m^2}{\lambda_0 - \lambda}, 1, \dots, 1 \right)^{-1} \\ &= \text{diag} \left(\frac{\lambda_0 - \lambda}{\lambda_0 - \lambda - ik\beta^2\pi_1^2}, \dots, \frac{\lambda_0 - \lambda}{\lambda_0 - \lambda - ik\beta^2\pi_m^2}, 1, \dots, 1 \right). \end{aligned}$$

Therefore

$$\lim_{\lambda \rightarrow \lambda_0} E_0^{-1} = P_0^\perp = \mathbb{I} - P_0. \quad (15)$$

Furthermore

$$E_0^* E_0^{-1} = \text{diag} \left(\frac{\lambda_0 - \lambda + ik\beta^2\pi_1^2}{\lambda_0 - \lambda - ik\beta^2\pi_1^2}, \dots, \frac{\lambda_0 - \lambda + ik\beta^2\pi_m^2}{\lambda_0 - \lambda - ik\beta^2\pi_m^2}, 1, \dots, 1 \right)$$

which gives us the limit

$$\lim_{\lambda \rightarrow \lambda_0} E_0^* E_0^{-1} = P_0^\perp - P_0 = \mathbb{I} - 2P_0. \quad (16)$$

From these limits we get

$$\begin{aligned} S(\lambda_0) &= - \left[\mathbb{I} - 2P_0 + ik_0\beta^2 Q_0 P_0^\perp \right] \sum_{s=0} (ik_0\beta^2 Q_0 P_0^\perp)^s \\ &= -\mathbb{I} + 2P_0 - 2 \sum_{s=1} (ik_0\beta^2 P_0^\perp Q_0 P_0^\perp)^s \\ &= -\mathbb{I} + 2P_0 + O(\beta^2). \end{aligned} \quad \square$$

This formula appears to imply that there may be non-zero transmission in the case of zero connection between the rays. Actually the transmission coefficients are not continuous with respect to λ uniformly in β [3, 23]. The physically significant parameters of the system are obtained by averaging as functions of λ over the Fermi distribution so that there is no transmission for $\beta = 0$.

Corollary 1 *If λ_0 is an eigenvalue of \mathcal{L} such that $P_0 = \mathbb{I}$ then the above formula is independent of β , ie.*

$$S(\lambda_0) = \mathbb{I}$$

Consequently, when we have pure reflection at an eigenvalue of the unperturbed operator, we have pure reflection regardless of the strength of the interaction between the rays and the compact domain.

3 Simple models

In [22] the authors discuss the case where Ω is the unit disc in R^2 and there are four one-dimensional wires attached at the points $\varphi = 0, \pi, \pm\pi/3$. The dynamics on Ω is given, using polar coordinates (r, θ) , by the dimensionless Schrödinger equation

$$-\Delta\Psi + [V_0 + \varepsilon r \cos(\theta)]\Psi = \lambda\Psi \quad (17)$$

on the domain with Neumann boundary conditions at the boundary:

$$\left. \frac{\partial \Psi}{\partial n} \right|_{r=1} = 0.$$

The dimensionless magnitude ε of the governing field is chosen so that the eigenfunction corresponding to the second smallest eigenvalue has only two zeroes on the boundary of the unit circle which divide the circumference in the ratio 2 : 1. It is then easy to see that by rotating the potential V one may redirect the quantum current from the wire attached to the point $\varphi = 0$ to any other wire with all of the other wires blocked [22].

The analysis in this case is similar to the analysis given above except there is now only a logarithmic singularity in the Greens function and the Krein formula for infinite deficiency indices [18, 24] and infinite-dimensional Rouchet theorem [12] play a central rôle. A large amount of the calculation was done using Mathematica.

In [15], using the above asymptotic formula for the scattering matrix to choose appropriate parameters, the author discusses the case where Ω is simply a one-dimensional ring and there is an angle of $\pi/2$ between the rays—see figure 2. a). By applying a uniform field to the ring, $q = 0$ for the open state and $q = -3$ for the closed state, it is easy to see that a switching effect is produced where the Fermi energy is assumed to correspond to the smallest eigenvalue of the unperturbed operator on the ring, ie. $\lambda_0 = 1$. See also [7] where a similar construction is considered.

Another possibility is to consider a device—see figure 2.b), the angle be-

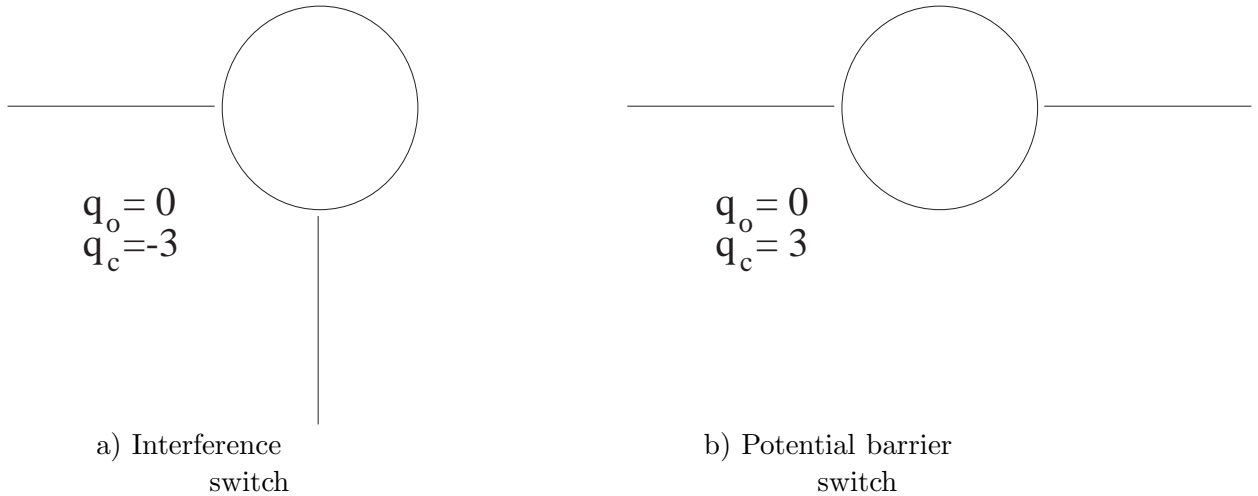


figure 2.

tween the rays is now π —with similar parameters where now we switch the current by raising a potential barrier, $q = 0$ for the open state and $q = 3$ for the closed state, instead of using interference effects. Clearly, unlike the first case, the efficiency of such a switch will be limited by tunneling.

A more detailed discussion of the properties of these two models (including plots of the averaged conductance in the closed, $\hat{\sigma}_c$, and open, $\hat{\sigma}_o$, states) is

presented in [16]. Here we just present the main observations, viz. for both switches the open state—possibly due to tunneling effects—is more difficult to achieve; and in the limit of small β , the properties of the switches improve. This is probably due to the fact that weak coupling between the ring and rays improves the open state of the switches. On the other hand, in the limit $\beta \rightarrow 1$, the ratio $\hat{\sigma}_c/\hat{\sigma}_o$ for the second example rapidly decreases to a bound due to tunneling which may be calculated from the transmission coefficient

$$\lim_{\tau \rightarrow 0} \left. \frac{\hat{\sigma}_c}{\hat{\sigma}_o} \right|_{\beta=1} \approx 4.57 \times 10^3.$$

The first switch does not have this bound and consequently for sufficiently low temperature or small radius (see first footnote) we conjecture that it will have better properties.

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